# IMPLEMENTATION OF LANDAU-FLUID CLOSURES FOR TOROIDAL SIMULATIONS IN BOUT++*

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# Simulations of tokamak (and other MFE) edge plasmas need to go beyond collisional (Braginskii) models

- Kinetic effects are important in the tokamak edge
- Gyro-Landau-fluid (GLF) approach is a way to incorporate some kinetic effects into fluid simulation codes such as BOUT++
- Radial inhomogeneities and large relative perturbation amplitudes necessitate a non-Fourier implementation of the Landau-fluid (LF) closure operators

- Related work at this workshop:
  - S.S. Kim: Gyro-Fluid Simulations using BOUT GLF Code (Friday 9.30am)
  - P. W. Xi: Gyrofluid Simulations on KBM and ELMs using BOUT++ (Thursday, 11.10am)
  - T. Xia: Six-Field Two-Fluid Simulations (Thursday, 2pm)

# The Landau-fluid (LF) closure operators are highly nonlocal in configuration space

- 1D (e.g., parallel) collisionless closure phase-mixing:
  - $\gamma \propto -|k|\, v_{\rm th}$
  - e.g., 3-moment model (collisionless: Hammett-Perkins, PRL '90):

$$\tilde{Q}_k \approx -\alpha n_0 v_{\rm th} \frac{1}{|k|}\left(ik\tilde{T}_k\right) \quad \Longleftrightarrow \quad \tilde{Q}\left(z\right) \approx \int\limits_{-\infty}^{\infty} dz' G(z-z')\tilde{T}\left(z'\right)$$

$$G(z) \quad = \quad \frac{\alpha}{\pi} n_0 v_{\rm th} \frac{1}{z}$$

  - with collisions (Beer-Hammett, Phys. Plasmas '96):

$$\tilde{Q}_k \approx -\frac{8 n_0 v_{\rm th}^2 ik\tilde{T}_k}{\sqrt{8\pi}\,|k|\, v_{\rm th} + (3\pi - 8)\,\nu_s}$$

- If spatially homogeneous closure model can be used, the LF operators are easy to represent and efficient to calculate in Fourier ($k_{\shortparallel}$) space.

# The LF closure operators for edge must deal with spatial inhomogeneities

- Example: toroidal Landau-fluid ($|\omega_d|$) closure:
- e.g., Beer-Hammett '96, 3+1 equations:

$$\frac{dp_{\parallel}}{dt} = \mathrm{stuff} - i\omega_d\left(7p_{\parallel} + p_{\perp} - 4n\right) - 2\left|\omega_d\right|\left(\nu_1 T_{\parallel} + \nu_2 T_{\perp}\right)$$

- $\omega_d$ defined by

$$\begin{aligned} i\omega_d \Psi &= v_d \hat{\mathbf{v}}_d \cdot \nabla_{\perp} \Psi \\ &= \frac{1}{2(T_{\mathrm{norm}} B_0)}\left[\frac{T_{\perp}}{B_0}\hat{\mathbf{b}} \times \nabla B_0 \cdot \nabla + T_{\parallel}\hat{\mathbf{b}} \times \left(\hat{\mathbf{b}} \cdot \nabla \hat{\mathbf{b}}\right) \cdot \nabla\right]\Psi \end{aligned}$$

  - In the edge, $T_{\perp}$ and $T_{\parallel}$ have significant spatial variations due to
    - equilibrium profile variation
    - finite amplitude perturbations

# Computation of the LF operators becomes challenging when significant spatial inhomogeneities are present

- Operators are no longer local in $k$ space
  - Fourier-based computation inefficient
- LF operators intrinsically nonlocal in configuration space $\rightarrow$ mesh-based discretization schemes used for derivatives (finite difference, volume, element, etc.) are not directly applicable.
- Straightforward direct approach:
  - discretize configuration-space kernel
  - aplply by direct convolution or matrix multiplication
  - computationally expensive; $N_g^2$ scaling [vs. $N_g \log(N_g)$ for local-$k$ Fourier]
- ACCURATE APPROXIMATIONS ARE POSSIBLE THAT CAN BE IMPLEMENTED WITH FOURIER-LIKE SCALING.

# Approximation by a sum of Lorentzians allows for computation using efficient sparse linear solvers

- Lorentzians in $k$ space are inverses of Helmholtz operators in real space
- Could provide very efficient way to implement nonlocality

- Consider

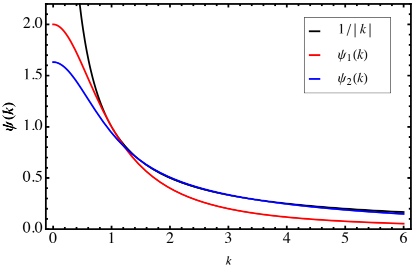
$$\frac{1}{|k|^\gamma} \approx \psi_\infty(k,\alpha,\gamma) \approx \sum_{n=-\infty}^{\infty} \frac{\alpha^{\gamma n}}{k^2 + \alpha^{2\gamma n}},\ 0 < \gamma < 2$$

- Converges pointwise; satisfies $\psi_\infty(\alpha k, \alpha) = \alpha^{-\gamma}\psi_\infty(k,\alpha)$
- Each individual component of the sum has the correct parity.
- With the above scaling of the height and width, different terms approximately "fill in" different parts of the $1/|k|$ curve
- Suggests an approximation by a simple truncation.

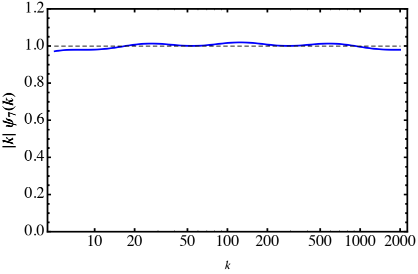
# Simple truncated sum of Lorentzians is very accurate, even with few terms

$$\frac{1}{|k|} \approx \psi_N\left(k, \alpha, \beta, k_0\right) \approx \beta \sum_{n=0}^{N-1} \frac{\alpha^n k_0}{k^2 + \left(\alpha^n k_0\right)^2}$$

$\psi_N\left(k\right)$ - 1 and 2 terms




$|k|\,\psi_7\left(k\right)$ - 7 terms



# Systematic collocation analysis $\rightarrow$ improved fits: collisionless

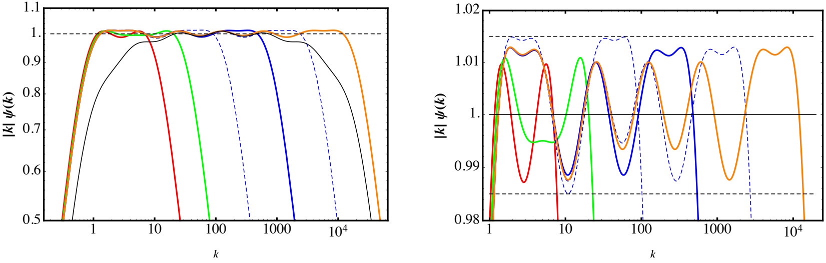
- Collisionless - good (near best) fit is of the form

$$1/|k| \approx \sum_{n=0}^{N-1} \frac{\zeta_n \alpha^n \kappa_0}{k^2 + (\alpha^n \kappa_0)^2},$$

- Match exact and approximate forms at collocation points
  - $k = k_n$, $k_n = \alpha^{n-1}\kappa_0$, $n = 1, 3, \ldots, N-2$
  - shift end collocation points: $k_0 = \kappa_0/\eta$, $k_N = \eta\alpha^{N-1}\kappa_0$.
- $\rightarrow$ matrix problem that can be handled e.g., by Mathematica

# Systematic collocation analysis → improved fits: collisionless

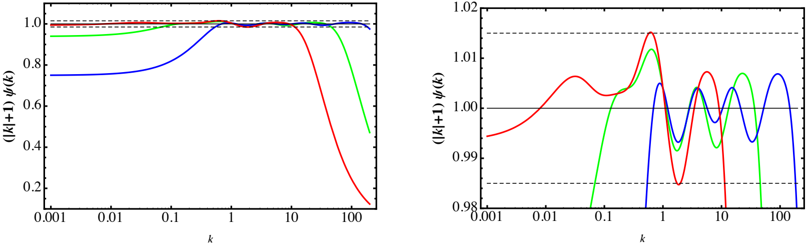
- Extends spectral range of good fit by ~10-100 for given $N$, $\alpha$.
- Improved fits vs. original fit
- Spectral range of good fit: 7, 20, 80, 400, 2000, 10000



# Systematic collocation analysis → improved fits: collisional

$$\frac{1}{(|k|+1)} \approx \sum_{n=-M}^{N} \frac{\zeta_n}{k^2+\alpha^{2n}},$$

- Collocation points: $k_n = \alpha^n$, $n = -M, \ldots, N-1$, $k_N = \eta\alpha^N$.
- 5 terms → good fit over spectral range $\approx 400$, $\forall\, k\lambda_{\mathrm{mfp}}$.
- $\alpha = 3;\ N+M+1 = 5$,



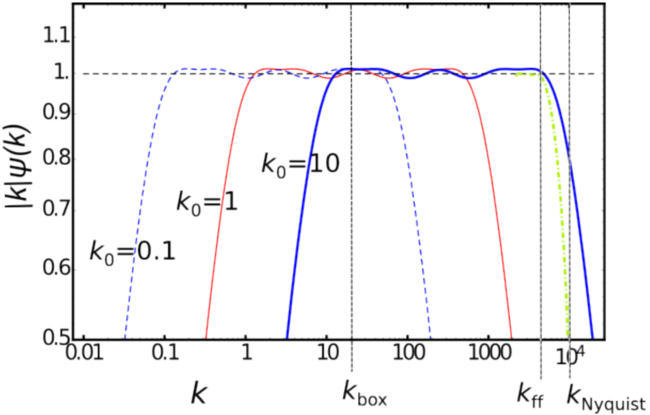
# Implementation is by replacement of Lorentzians in wavenumber space by Helmholtz-equation solves

- Solve via a tridiagonal (for 2-point differences) or banded (for higher-order differences) matrix solution
- Direct solvers work well
  - the matrices are well conditioned
  - parallelizeable along direction of solve
- Sum the results of the matrix solves

$$\Psi(z) \approx \sum_n \zeta_n \alpha^n \kappa_0 \left[ (\alpha^n \kappa_0)^2 - \frac{\partial^2}{\partial z^2} \right]^{-1} S(z)$$

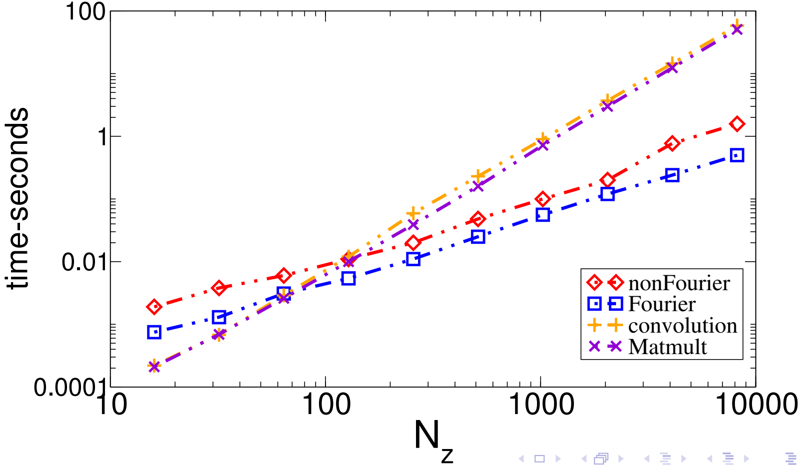
# Normalizing wavenumber $k_0$ must be chosen to have region of good fit overlap with resolved modes

- Choose $k_0$ so that
  - $k_{\rm box}$ is to right of left boundary of good fit
  - $k_{\rm ff}$ is to left of right boundary of good fit



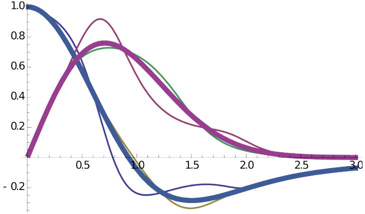
# Sum-of-Lorentzians method has similar computational scaling to Fourier

- Scales as $N_z \log(N_z)$, c.f. $N_z^2$ for direct convolution or matrix multiplication.
- Crossover point is at $N_z \approx 128 \Rightarrow$ advantage for $N_z \gtrsim 200$.



# Using sum of Lorentzians approximation preserves Hammett-Perkins '90 LF response functions

- Implemented Mathematica scripts; reproduced HP90 calculations,
- modified to also use sum of Lorentzians for $1/|k|$.




$R = R_4\,(k/k_0),$
$k_0 = 1,\ 10,\ 100.$

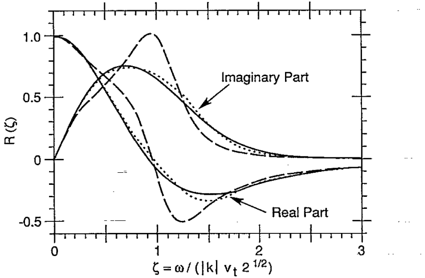
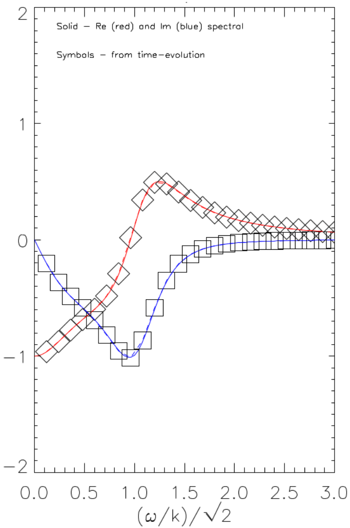


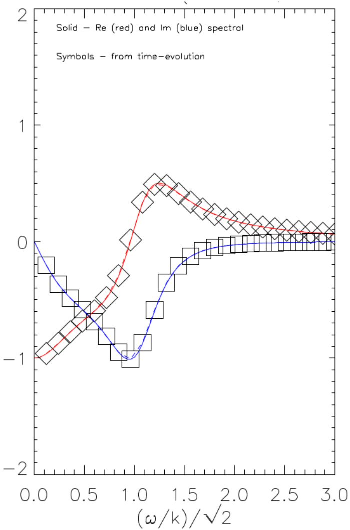

FIG. 1. The real and imaginary parts of the normalized response function $R(\zeta) = -\tilde{n}T_0/n_0e\tilde{\phi}$ vs the normalized frequency $\zeta$. The solid lines are the exact kinetic result for a Maxwellian, $R(\zeta) = 1 + \zeta Z(\zeta)$. The dashed lines are from the three-moment fluid model with $\Gamma = 3$, $\mu_1 = 0$, and $\chi_1 = 2/\sqrt{\pi}$. The dotted lines are from the four-moment model.

# Implementation using sum of Lorentzians approximation in BOUT++ preserves collisionless LF response functions

non-Fourier




Fourier



# The LF terms have been implemented in BOUT++

- $|k_{||}|$ terms implemented using existing parallel "Laplace" solver
  - Has correct offset periodic parallel boundary conditions
- $|\omega_d|$ terms implemented using modification of existing perpendicular Laplace solver(s)
  - Existing solver solves $\left(c_1\nabla_\perp^2 + \frac{1}{c_2}\nabla_\perp c_2.\nabla_\perp + c_3\right)\Psi = S$
  - Modify to solve $\left[\alpha^2 k_{\phi 0}^2 - \left(\hat{\mathbf{V}}_\mathbf{d}\cdot\nabla\right)^2\right]\Psi = S$
- Radial inhomogeneities in $\nabla B$ and curvature drifts can be included via the manifestly conservative dissipative form:

$$|\mathbf{k}.\mathbf{V}_\mathbf{d}(x)|\,\Psi = \nabla\cdot\left[\hat{\mathbf{V}}_\mathbf{d}\sqrt{\mathrm{V}_\mathbf{d}}\frac{1}{\left|\mathbf{k}.\hat{\mathbf{V}}_\mathbf{d}\right|}\sqrt{\mathrm{V}_\mathbf{d}}\left(\hat{\mathbf{V}}_\mathbf{d}\cdot\nabla\Psi\right)\right]$$

# Toroidal Landau-fluid ($|\omega_d|$) closure

- Definition of $i\omega_d$

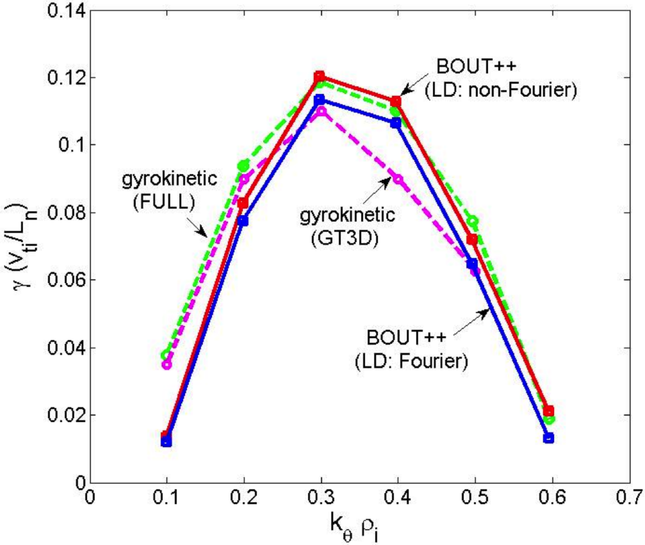
$$\begin{aligned} i\omega_d \Psi &= i\mathbf{V}_d \cdot \mathbf{k}_\perp \Psi \\ &= \frac{1}{2(T_{\text{norm}} B_0)} \left[ \frac{T_{\perp 0}}{B_0} \hat{\mathbf{b}} \times \nabla B_0 \cdot \nabla + T_{\shortparallel 0} \hat{\mathbf{b}} \times \left( \hat{\mathbf{b}} \cdot \nabla \hat{\mathbf{b}} \right) \cdot \nabla \right] \Psi \end{aligned}$$

- $T_{\perp 0} = T_{\perp 0}(\psi)$, $T_{\shortparallel 0} = T_{\shortparallel 0}(\psi)$; - eventually will need to generalize to finite amplitude
- Decompose $\mathbf{V}_d$ and $\nabla\Psi$ into components

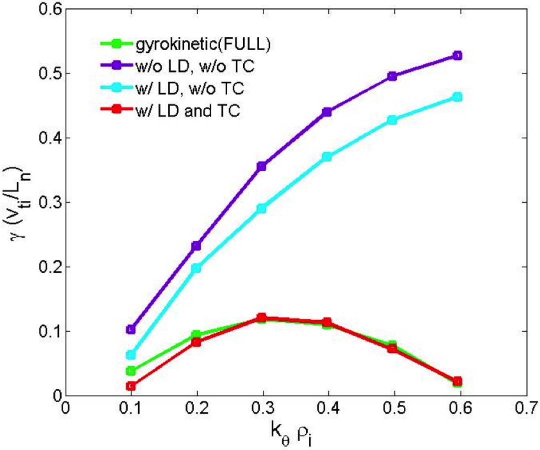
$$\begin{aligned} \mathbf{V}_d &= V_d^i \mathbf{e}_i \\ \nabla\Psi &= \mathbf{e}^i \partial_i \Psi \\ \mathbf{V}_d \cdot \nabla\Psi &= V_d^i \partial_i \Psi \end{aligned}$$

$$\left\{ \left[ \left( V_d^\phi \right)^2 k_\phi^2 - \left( V_d^\psi \right)^2 \partial_\psi^2 - 2i V_d^\psi V_d^\phi k_\phi \partial_\psi \right] + \alpha^2 \left( V_{d0} \right)^2 k_{\phi 0}^2 \right\} \Psi = S$$

# Good agreement is achieved with previous calculations for ITG instability frequencies and growth rates



# The Landau-Fluid terms are essential for agreement of the GLF toroidal ITG linear growth rates with gyrokinetic results



# Conclusions

- We have developed a new non-Fourier method for the calculation of Landau-fluid operators.
- Useful for situations with large (including background) spatial inhomogeneities.
- Good accuracy (relative error $\lesssim 1.5\%$ over wide spectral range) is readily achievable with 5 terms for all $k\lambda_{\mathrm{mfp}}$.
- Computational cost has value and scaling similar to Fourier method.
- Considerable advantage over direct convolution or matrix multiplication for $N_g \gtrsim 200$.
- Implemented for parallel ($|k_{\shortparallel}|$) and toroidal ($|\omega_{\mathrm{d}}|$) LF operators in BOUT++
- Good agreement is achieved with previous calculations for ITG instability frequencies and growth rates.

# Near-term ongoing work: Nonlinear verification with all "known" GLF physics (see APS-DPP talk)

- Implementation of Dorland nonlinear phase-mixing closure:
  - Same machinery as for $|\omega_d|$ closure ($\mathbf{v_d} \rightarrow \hat{\nabla}_\perp^2 \mathbf{V}_\Phi$)
- GLF model for zonal flows:
  - Based on work by Rosenbluth, Hinton & Waltz; Beer & Hammett; Sugama, Watanabe & Horton.
  - Some reworking and inclusion of finite banana width as well as FLR (can't separate for typical tokamak edge or tight aspect ratio)
  - Include collisions.
- Extend implementation of $\perp$ closure terms to (completely) non-Fourier solvers.
- Extensions of closures to large amplitude:
  - Still phase mixing, but can include some inhomogeneity effects in closures.